

Formaldehyde

50-00-0 | DTXSID7020637

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.40e-01

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methanol</div> <div>Measured: 0.44</div> <div>Predicted: 4.42e-01</div>	<div>Image not found</div> <div>Ethyleneimine</div> <div>Measured: 0.78</div> <div>Predicted: 6.20e-01</div>	<div>Image not found</div> <div>Ethanol</div> <div>Measured: 0.2</div> <div>Predicted: 3.50e-01</div>
<div>Image not found</div> <div>Acetic acid</div> <div>Measured: 0.0</div> <div>Predicted: 3.79e-01</div>	<div>Image not found</div> <div>Acetamide</div> <div>Measured: 0.7</div> <div>Predicted: 6.47e-01</div>	